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# Contents

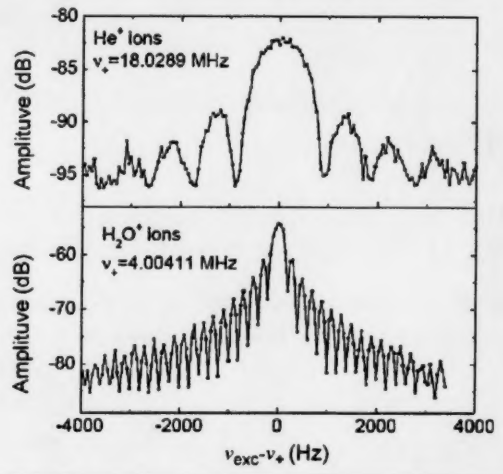
## Regular articles

*1–5*

**A broad-band FT-ICR Penning trap system for KATRIN**

M. Ubieto-Díaz, D. Rodríguez, S. Lukic, Sz. Nagy, S. Stahl, K. Blaum

Two three-electrode cylindrical Penning traps using the Fourier-Transform Ion-Cyclotron-Resonance detection technique in order to measure the concentration of unwanted species will be installed in the KATRIN beamline. The system is presently under commissioning at the Max-Planck-Institute for Nuclear Physics in Heidelberg.

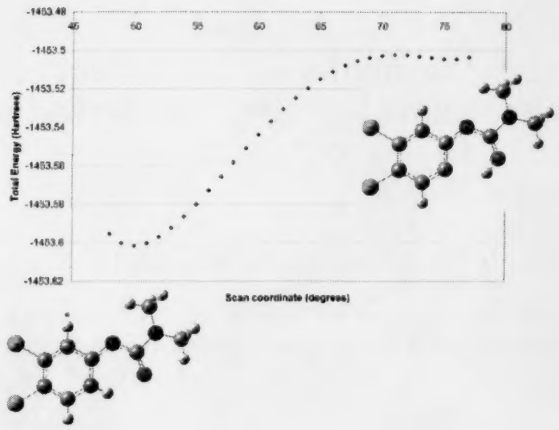



*6–15*

**Exploring rearrangements along the fragmentation pathways of diuron anion: A combined experimental and computational investigation**

Basem Kanawati, Mourad Harir, Philippe Schmitt-Kopplin

Successive two 1,3 $H^+$ shifts of the marked Proton $^*H^+$ are responsible for the elimination of dimethylamine from the Diuron anion (left). DFT studies exclude the possibility of a 1,5 proton shift in a Mclafferty like type of rearrangement. The PES shows the unfavourable energy demand for the forbidden 1,5 proton shift.

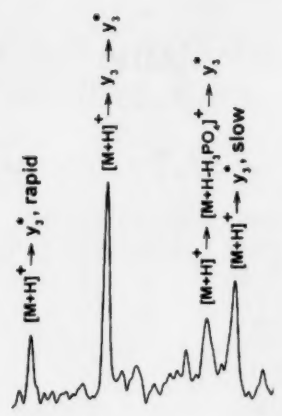



*16–21*

**Utility of reaction intermediate monitoring with photodissociation multi-stage ($MS^n$) time-of-flight mass spectrometry for mechanistic and structural studies: Phosphopeptides**

Jeong Hee Moon, Young Sik Shin, Myung Soo Kim

Photoexcitation inside a high voltage cell splits a dephosphorylated sequence peak ($y_3^*$) into several components. $y_3^*$ is formed mainly via $[M + H]^+ \rightarrow y_3 \rightarrow y_3^*$.

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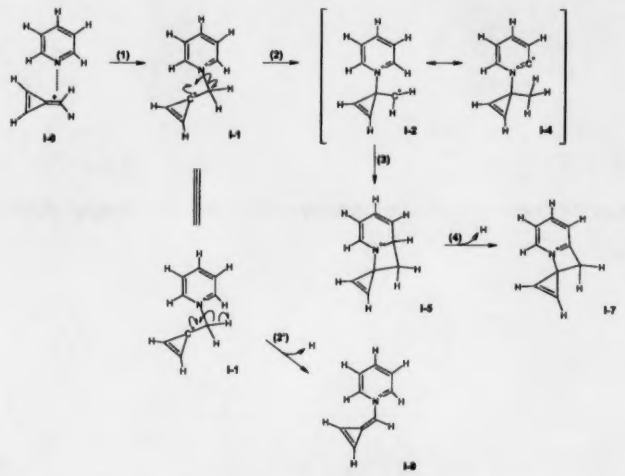
doi:10.1016/S1387-3806(09)00331-5

*22–35*

**Condensation reaction of $C_4H_4^+$ with pyridine**

C.Q. Jiao, J.A. Boatz, C.A. DeJoseph Jr., A. Garscadden

Quantum chemistry theory and FTMS experiments on the reactions of $C_4H_4^+$ with $C_5H_5N$ that show $H^+$ transfer, charge transfer and condensation with H-elimination.

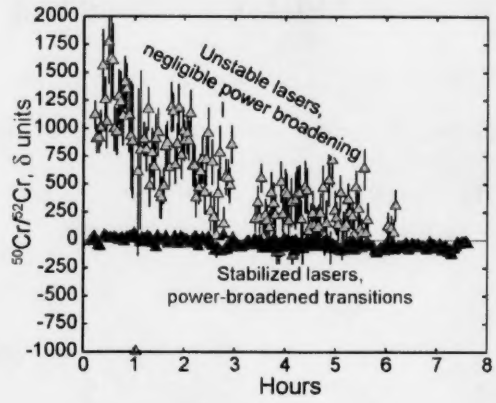


*36–43*

**Resonance ionization mass spectrometry for precise measurements of isotope ratios**

Jonathan Levine, Michael R. Savina, Thomas Stephan, Nicolas Dauphas, Andrew M. Davis, Kim B. Knight, Michael J. Pellin

We measure isotope ratios with sub-percent precision by resonance ionization mass spectrometry, using stabilized resonance lasers and power-broadened optical transitions.

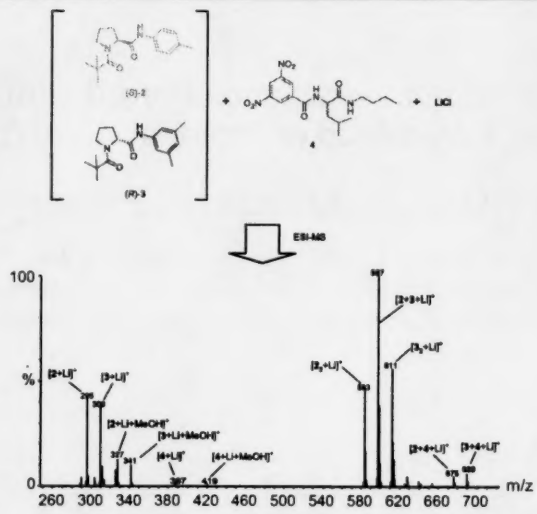



*44–50*

**Chiral recognition and enantiomer assays of *N*-(3,5-dinitrobenzoyl) amino acid derivatives using electrospray ionization–mass spectrometry**

Chengli Zu, Jonathan A. Woolfolk, Michael E. Koscho

We performed chiral recognition and enantiomer assays of *N*-(3,5-dinitrobenzoyl)amino acid derivatives in the gas phase using electrospray ionization/mass spectrometry (ESI/MS).

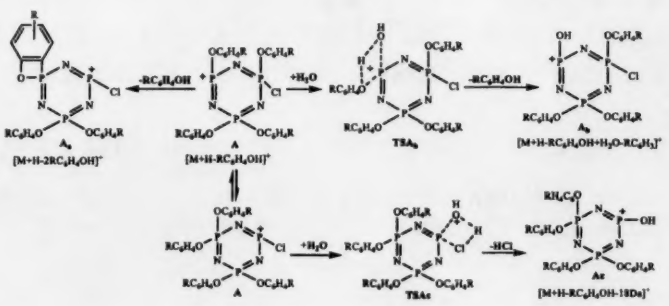



*51–57*

**Electrospray ionization multistage tandem mass spectrometry of penta- and hexa-substituted aryloxycyclotriphosphazenes**

Zhiyu Ju, Yong Ye, Donghui Wei, Ruyi Zou, Yufen Zhao

Several penta- and hexa-substituted aryloxycyclotriphosphazenes were synthesized and investigated by electro spray ionization tandem mass spectrometry (ESI-Ms$^n$).

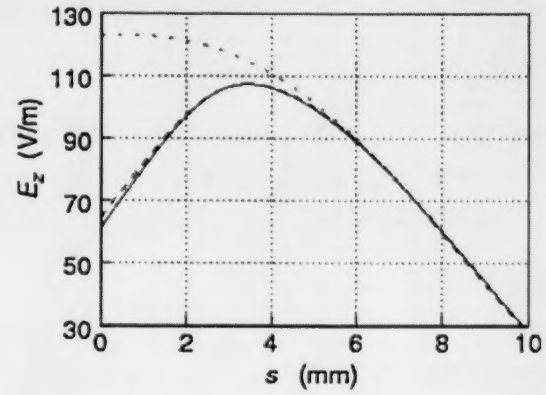


*58–67*

**Off-axis field approximations for ion traps with apertures**

Madhurima Chattopadhyay, Atanu K. Mohanty·

This paper presents analytical approximations for the fields in ion traps with apertures. $E_Z$ computed numerically (solid line) and by our approximation (dashed line).

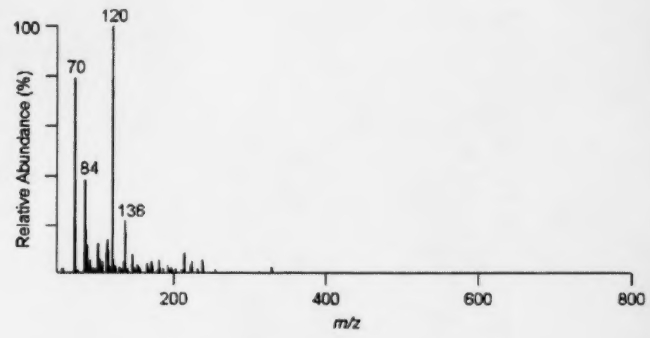



*68–74*

**Fragmentation of peptides with intra-chain disulfide bonds in triple quadrupole mass spectrometry and its quantitative application to biological samples**

Yun Chen, Shanlei Qiao, Ce Wang

Generation of abundant immonium ions in product ion spectrum of peptides with intra-chain disulfide bonds.

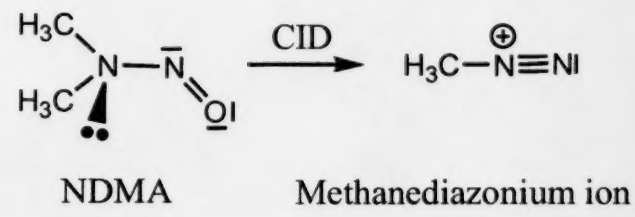



*75–83*

**Collision induced dissociation of protonated N nitrosodimethylamine by ion trap mass spectrometry: Ultimate carcinogens in gas phase**

Natalia Kulikova, Michael Baker, Wojciech Gabryelski

Gas phase ion chemistry of a potent carcinogen N-nitrosodimethylamine (NDMA) has been found to produce methanediazonium ion which is considered the ultimate carcinogen in metabolic pathway of NDMA in biological systems.

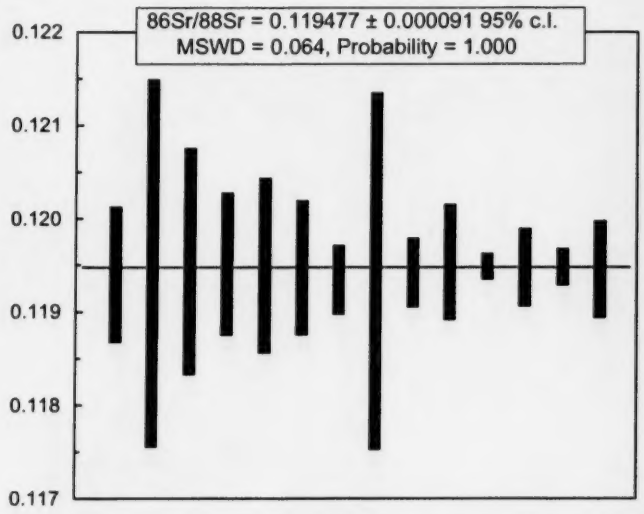



*84–91*

**Rayleigh's distillation law and linear hypothesis of isotope fractionation in thermal ionization mass spectrometry**

Giancarlo Cavazzini

The relationship which exists between Rayleigh's distillation process and the linear hypothesis of instrumental isotope fractionation in thermal ionization-source mass spectrometry is investigated.



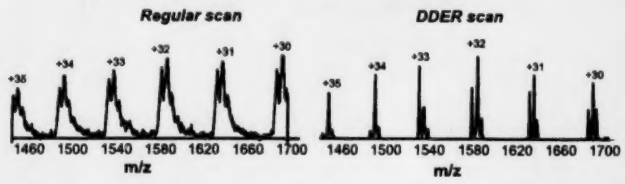
## Short communication

*92–95*

**Improved mass analysis of intact proteins by ion trap instrument on a chromatographic time scale via data-dependant enhanced resolution scan**

Gang Hao, Jane Gu

A novel method that improves the mass spectra resolution for multiply charged protein ions on ion trap instruments.



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